

Taurocyamine

543-18-0 | DTXSID10202654

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.60

Global applicability domain: Inside

Local applicability domain index: 4.11e-01

Confidence level: 5.44e-01

Nearest Neighbors from the Training Set

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N<sup>2</sup>-Acetyl-L-aspartamide

Measured: -2.41

Predicted: -2.30

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N<sup>2</sup>-Acetyl-L-alpha-glutamine

Measured: -2.47

Predicted: -2.10

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Isocytosine

Measured: -0.990

Predicted: -1.02

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Propanenitrile, 3,3'-  
(nitrosoimino)bis- (9CI)

Measured: 0.08

Predicted: 1.13e-02